

Glycine, N,N-dimethyl-
1118-68-9 | DTXSID6074336

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: $2.38\text{e-}12 \text{ cm}^3/\text{molecule}\cdot\text{sec}$

Global applicability domain: Inside

Local applicability domain index: $6.53\text{e-}01$

Confidence level: $8.99\text{e-}01$

Nearest Neighbors from the Training Set

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Methyl 2-hydroxypropanoate

Measured: $2.80\text{e-}12$

Predicted: $3.16\text{e-}12$

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Butanoic acid

Measured: $2.40\text{e-}12$

Predicted: $2.30\text{e-}12$

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2-Methylpropanoic acid

Measured: $2.00\text{e-}12$

Predicted: $1.95\text{e-}12$

Image not found

Ethyl lactate

Measured: $3.90\text{e-}12$

Predicted: $4.80\text{e-}12$

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Propionic acid

Measured: $1.22\text{e-}12$

Predicted: $1.27\text{e-}12$